

SPHERE PACKINGS III

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1. INTRODUCTION AND REVIEW

This paper is a continuation of the first two parts of this series ([I],[II]). It relies on the formulation of the Kepler conjecture in [F]. The terminology and notation of this paper are consistent with these earlier papers, and we refer to results from them by prefixing the relevant section numbers with I, II, or F. Around each vertex is a modification of the Voronoi cell, called the *V-cell* and a collection of quarters and quasi-regular tetrahedra. These objects constitute the *decomposition star* at the vertex. A decomposition star may be decomposed into *standard clusters*. By definition, a standard cluster is the part of the given decomposition star that lies over a given *standard region* on the unit sphere.

A real number, called the *score*, is attached to each cluster. Each star receives a score by summing the scores $\sigma(R)$ for the clusters R in the star. The scores are measured in multiples of a *point* (pt), where $pt \approx 0.055$. If every star scores at most $8\,pt$, then the Kepler conjecture follows.

The steps of the Kepler conjecture, as outlined in Part I, are

1. A proof that if all standard regions are triangular, the total score is less than $8\,pt$
2. A proof that the standard regions with more than three sides score at most $0\,pt$
3. A proof that if all of the standard regions are triangles or quadrilaterals, then the total score is less than $8\,pt$ (excluding the case of pentagonal prisms)
4. A proof that if some standard region has more than four sides, then the star scores less than $8\,pt$
5. A proof that pentagonal prisms score less than $8\,pt$

This paper completes the third of these steps.

The standard regions of the decomposition stars in the face-centered cubic and the hexagonal-close packings are regular triangles and quadrilaterals. These stars score exactly $8\,pt$. The local optimality results for hexagonal-close packings and face-centered cubic packings have been established in [II]. If the planar map is that of

a close packing, there are eight quasi-regular tetrahedra. To score 8 pt , the quasi-regular tetrahedra must be regular of edge length 2 [I.9.1]. Such decomposition stars are precisely those of the close packings. Conjecturally, all the decomposition stars have scores strictly less than 8 pt , so that various approximations may be introduced to prove the desired bounds.

The standard regions of pentagonal prisms are triangles and quadrilaterals (10 triangles and 5 quadrilaterals). The pentagonal prisms are the subject of the fifth step of the program.

Theorem 1. *Let D^* be a decomposition star whose combinatorial structure is not a pentagonal prism. Suppose that each standard region of D^* is a triangle or quadrilateral. Then the score of D^* is at most 8 pt . Equality is attained exactly when the decomposition of the unit sphere into standard regions coincides with that of a decomposition star in the face-centered cubic or hexagonal-close packing.*

The proof of Theorem 1 relies on many computer calculations. We make a list of combinatorial properties that a decomposition star must have for it to have a possibility of scoring more than 8 pt . We then make a computer search to find all decompositions of the unit sphere into triangles and quadrilaterals that satisfy all the properties on the list. The computer search produces an explicit list containing nearly 2000 combinatorial types.

For each of these combinatorial arrangements of triangles and quadrilaterals, we have a nonlinear optimization problem: maximize the score over the space of all decomposition stars D^* with the given combinatorial arrangement. It is not necessary to solve this optimization problem. It is sufficient to establish an upper bound of 8 pt . To do this, we define a *linear relaxation* of the original problem, that is, a linear programming problem whose solution strictly dominates the global maximum of the original nonlinear problem. This gives an upper bound on the linear problem, which is usually less than 8 pt .

In some cases, this procedure leads to a bound greater than 8 pt , and further analysis will be required.

One advantage of our method of linear relaxation is that the verification of the bounds is particularly simple. If the linear relaxation asks to maximize $c \cdot x$ subject to the system of linear inequalities $Ax \leq b$ and $x \geq 0$, then duality theory produces a vector z with nonnegative entries such that $c \leq zA$. To verify the bound of 8 pt , it is enough to check that $c \leq zA$, $z \geq 0$, and $z \cdot b < 8\text{ pt}$ (because then $c \cdot x \leq zAx \leq z \cdot b < 8\text{ pt}$).

Many of the linear inequalities that were used in the linearly relaxed optimization problems were obtained as follows. We use numerical methods to find a convex polygon containing the set of ordered pairs

$$(\text{dih}(S), \sigma(S))$$

as S ranges over quasi-regular tetrahedra. The edges of the polygon give linear inequalities relating the dihedral angles to the score σ . More generally, additional inequalities are obtained by considering polygons that contain the ordered pairs

$$(\text{dih}(S), \sigma(S) - \lambda \text{sol}(S)),$$

for appropriate constants λ . Similar inequalities are obtained for quadrilateral regions.

We must remember that ultimately we are dealing with a nonlinear optimization problem that is larger, by a considerable order, than what is conventionally thought to be solvable by exact methods. The domain of our optimization problem has many components, and the dimension varies from component to component. Even the magnitude of the problem is poorly understood. The best-known bound on the dimension of the components is about 155 dimensions. Components of interest frequently have more than 35 dimensions. The decomposition into standard regions gives the problem an aspect of separability. Nevertheless, certain complications will have to be tolerated.

The biggest weakness of this method is that the output from the computer search for the combinatorial arrangements of triangles and quadrilaterals is not easily checked for errors. The algorithm is described in some detail in Section 9, but the only assurance that no cases have been skipped comes through a careful reading of the computer code. It would be advantageous to have a more transparent proof of the results of this section.

This paper is supplemented by an appendix giving further details of the combinatorial arrangements. Additional details about these calculations, including the full source code for all of the computer verifications of this paper, can be found in [H2].

The outline of this paper was developed at the University of Chicago during the summer of 1994. I would like to thank to P. Sally for making computer resources and other facilities available to me during my stay in Chicago, and for his encouragement with this work. I would also like to give special thanks to S. Ferguson for many helpful discussions concerning this topic. His investigations have led to a number of improvements in the results presented here.

2. GEOMETRIC CONSIDERATIONS

2.1. We will call a standard cluster over a quadrilateral region a *quad cluster*. The four vertices of the quad cluster whose projections to the unit sphere mark the extreme points of the quadrilateral region will be called the *corners* of the cluster. We call the four angles of the standard region associated with the quad cluster its *dihedral* angles.

The rules defining the score have undergone a long series of revisions over the last several years. The formulation used in this paper is described in [F].

Lemma 2.2. *A quadrilateral region does not enclose any vertices of height 2.51 or less.*

Proof. Let v_1, \dots, v_4 be the corners of the quad cluster, and let v be an enclosed vertex of height at most 2.51. We cannot have $|v_i - v| \leq 2.51$ for two different vertices v_i , because two such inequalities would partition the region into two separate standard regions instead of a single quadrilateral region. We apply I.4.3 to simplify the quad cluster. (Lemma I.4.3 assumes the existence of another enclosed

vertex v' , but it can be omitted both from the statement of the Lemma and from the proofs without affecting matters.) Then I.4.3 allows us to assume

$$|v_i - v_{i+1}| = 2.51, \quad |v_i| = 2, \quad |v| = 2.51,$$

for $i = 1, \dots, 4$. Reindexing and perturbing v as necessary, we may assume that $2 \leq |v_1 - v| \leq 2.51$ and $|v_i - v| \geq 2.51$, for $i = 2, 3, 4$. Moving v , we may assume it reaches the minimal distance to two adjacent corners (2 for v_1 or 2.51 for v_i , $i > 1$). Keeping v fixed at this minimal distance, perturb the quad cluster along its remaining degree of freedom until v attains its minimal distance to three of the corners. This is a rigid figure. There are four possibilities depending on which three corners are chosen. Pick coordinates to show that the distance from v to the remaining vertex violates its inequality. \square

3. FUNCTIONS RELATED TO THE SCORE

Set $\zeta^{-1} := \text{sol}(S(2, 2, 2, 2, 2, 2)) = 2 \arctan(\sqrt{2}/5)$. The constant ζ is related to the other fundamental constants by the relations $pt = 2/\zeta - \pi/3$ and $\delta_{oct} = (\pi - 2/\zeta)/\sqrt{8}$. Rogers's bound is $\sqrt{2}/\zeta \approx 0.7796$.

We consider the functions $\sigma_\lambda(R) := \sigma(R) - \lambda \zeta \text{sol}(R) pt$, for $\lambda = 0, 1$, or 3.2 , where R is a standard cluster. The constant 3.2 was determined experimentally. We will see that σ_1 has a simple interpretation. We write $\tau(R) = -\sigma_1(R)$. If D^* is a decomposition star with standard clusters $\{R\}$, set $\tau(D^*) = \sum_R \tau(R)$.

Lemma 3.1. $\tau(R) \geq 0$, for all standard clusters R .

Proof. If R is not a quasi-regular tetrahedron, or if it is but $\text{rad}(R) \geq 1.41$, then $\sigma(R) \leq 0$ and $\text{sol}(R) > 0$, so that the result is immediate (see I.9.17). Assume that R is a quasi-regular tetrahedron and $\text{rad}(R) \leq 1.41$. The result follows from Calculation 10.3.6, which asserts that $\Gamma(R) \leq \text{sol}(R)\zeta pt$. (Equality is attained only for the regular tetrahedron of edge 2.) \square

Lemma 3.2.

$$\sigma(D^*) = 4\pi\zeta pt - \tau(D^*).$$

Proof. Let R_1, \dots, R_k be the standard clusters in D^* . Then

$$\sigma(D^*) = \sum \sigma(R_i) + (4\pi - \sum \text{sol}(R_i))\zeta pt = 4\pi\zeta pt - \sum \tau(R_i).$$

\square

Since $4\pi\zeta < 22.8$, we find as an immediate corollary that if there are standard clusters satisfying $\tau(R_1) + \dots + \tau(R_k) \geq 14.8 pt$, then the score of the star is less than $8 pt$.

The function $\tau(R)$ gives the amount *squandered* by a particular standard cluster R . If nothing is squandered, then $\tau(R_i) = 0$ for every standard cluster, and the upper bound is $4\pi\zeta pt \approx 22.8 pt$. This is Rogers's bound on density. It is the unattainable

bound that would be obtained by packing regular tetrahedra around a common vertex with no distortion and no gaps. (More precisely, in the terminology of [H1], the score $s_0 = 4\pi\zeta pt$ corresponds to the *effective density* $16\pi\delta_{oct}/(16\pi - 3s_0) = \sqrt{2}/\zeta \approx 0.7796$, which is Rogers's bound.) Every positive lower bound on $\tau(R_i)$ translates into an improvement on Rogers's bound. To say that a decomposition star scores at most $8 pt$ is to say that at least $(4\pi\zeta - 8)pt \approx 14.8 pt$ are squandered.

4. SOME LINEAR CONSTRAINTS

This section gives some linear inequalities between $\sigma(R) - \lambda \text{sol}(R)\zeta pt$ and $\text{dih}(R)$.

Proposition 4.1. *Let R be a quad cluster. Let $\sigma(R)$ denote its score, let $\text{dih}(R)$ be one of the four dihedral angles of R , and let $\text{sol}(R)$ be the solid angle of the standard region of R . The following inequalities hold among $\text{dih}(R)$, $\text{sol}(R)$, and $\sigma(R)$:*

- 1: $\sigma(R) < -5.7906 + 4.56766 \text{dih}(R)$,
- 2: $\sigma(R) < -2.0749 + 1.5094 \text{dih}(R)$,
- 3: $\sigma(R) < -0.8341 + 0.5301 \text{dih}(R)$,
- 4: $\sigma(R) < -0.6284 + 0.3878 \text{dih}(R)$,
- 5: $\sigma(R) < 0.4124 - 0.1897 \text{dih}(R)$,
- 6: $\sigma(R) < 1.5707 - 0.5905 \text{dih}(R)$,
- 7: $\sigma(R) < 0.41717 - 0.3 \text{sol}(R)$,
- 8: $\sigma_1(R) < -5.81446 + 4.49461 \text{dih}(R)$,
- 9: $\sigma_1(R) < -2.955 + 2.1406 \text{dih}(R)$,
- 10: $\sigma_1(R) < -0.6438 + 0.316 \text{dih}(R)$,
- 11: $\sigma_1(R) < -0.1317$,
- 12: $\sigma_1(R) < 0.3825 - 0.2365 \text{dih}(R)$,
- 13: $\sigma_1(R) < 1.071 - 0.4747 \text{dih}(R)$,
- 14: $\sigma_{3.2}(R) < -5.77942 + 4.25863 \text{dih}(R)$,
- 15: $\sigma_{3.2}(R) < -4.893 + 3.5294 \text{dih}(R)$,
- 16: $\sigma_{3.2}(R) < -0.4126$,
- 17: $\sigma_{3.2}(R) < 0.33 - 0.316 \text{dih}(R)$,
- 18: $\sigma(R) < -0.419351 \text{sol}(R) - 5.350181 + 4.611391 \text{dih}(R)$,
- 19: $\sigma(R) < -0.419351 \text{sol}(R) - 1.66174 + 1.582508 \text{dih}(R)$,
- 20: $\sigma(R) < -0.419351 \text{sol}(R) + 0.0895 + 0.342747 \text{dih}(R)$,
- 21: $\sigma(R) < -0.419351 \text{sol}(R) + 3.36909 - 0.974137 \text{dih}(R)$.

Proposition 4.2. *Let R be a quad cluster. Let $\text{dih}_1(R)$ and $\text{dih}_2(R)$ be two adjacent dihedral angles of R . Set $d(R) = \text{dih}_1(R) + \text{dih}_2(R)$. The following inequalities hold between $d(R)$ and $\sigma(R)$.*

- 1: $\sigma(R) < -9.494 + 3.0508 d(R)$,
- 2: $\sigma(R) < -1.0472 + 0.27605 d(R)$,
- 3: $\sigma(R) < 3.5926 - 0.844 d(R)$,

Proposition 4.3.

- 1: $1.153 < \text{dih}(R)$,
- 2: $\text{dih}(R) < 3.247$.

Proof. Proposition 4.3 follows from interval arithmetic calculations based on the methods of [I]. The lower bound of 1.153 holds in fact for the dihedral angles of any standard cluster other than quasi-regular tetrahedra. \square

All of these inequalities have been proved by interval arithmetic methods by computer. An appendix gives a general description of the cases involved in the verification. Further details are available [H2].

5. TYPES OF VERTICES

The combinatorial structure of a decomposition star is conveniently described as a *planar map*. A planar graph is a graph that can be embedded into the plane or sphere. A planar map is a planar graph with additional combinatorial structure that encodes a particular embedding of the graph [T]. All our planar maps will be unoriented: we do not distinguish between a planar map and its reflection. Associated with a planar map are faces, (combinatorial) angles between adjacent edges, and so forth. Associated with each planar map L is a planar graph $G(L)$, obtained by forgetting the additional combinatorial structure. Each planar map has a dual L^* , obtained by interchanging faces and vertices. The faces of a planar map are in natural bijection with the vertices of L^* . We say that a face is an n -gon if the corresponding vertex in the dual L^* has degree n . The *boundary* of a face is an n -circuit in $G(L)$. The edges of the boundary are in natural bijection with the edges in L^* that are joined to the dual vertex of the face in L^* .

Associated with each decomposition star is a standard decomposition of the unit sphere, as described in Part I. We form a planar map L by associating with each standard region a face of L and with each edge of a standard region an edge of L . This paper is concerned with the special case of the Kepler conjecture in which every face of L is a triangle or quadrilateral.

We say that a vertex v of L has *type* (p, q) if there are exactly p triangular faces and q quadrilateral faces that meet at v . We write (p_v, q_v) for the type of v . The type of a vertex of the decomposition star is the type of the corresponding vertex in the planar map.

We use the following strategy in the proof of step 3 of the Kepler conjecture. The linear inequalities that were stated in Section 4 will be combined to give a bound on the score of the standard clusters around a given vertex of a given type. This bound will depend only on the type of the vertex. The bound comes as the solution to the linear programming problem of optimizing the sum of scores, subject to the linear constraints of Section 4 and to the constraint that the dihedral angles around the vertex sum to 2π . Similarly, we obtain a lower bound on what is squandered around each vertex.

This gives certain obvious constraints on decomposition stars. For example, if more than $(4\pi\zeta - 8)pt$ are squandered at a vertex of a given type, then that type of vertex cannot be part of a decomposition star scoring more than $8pt$. These relations between scores and vertex types will allow us to reduce the feasible planar

maps to an explicit finite list. For each of the planar maps on this list, we calculate a second, more refined linear programming bound on the score. Often, the refined linear programming bound is less than $8pt$.

This section derives the bounds on the scores of the clusters around a given vertex as a function of the type of the vertex. Define constants $\tau_{LP}(p, q)/pt$ by Table 5.1. The entries marked with an asterisk will not be needed.

(5.1)

$\tau_{LP}(p, q)/pt$	$q = 0$	1	2	3	4	5
$p = 0$	*	*	15.18	7.135	10.6497	22.27
1	*	*	6.95	7.135	17.62	32.3
2	*	8.5	4.756	12.9814	*	*
3	*	3.6426	8.334	20.9	*	*
4	4.1396	3.7812	16.11	*	*	*
5	0.55	11.22	*	*	*	*
6	6.339	*	*	*	*	*
7	14.76	*	*	*	*	*

Proposition 5.2. *Let S_1, \dots, S_p and R_1, \dots, R_q be the tetrahedra and quad clusters around a vertex of type (p, q) . Consider the constants of Table 5.1. We have*

$$\sum^p \tau(S_i) + \sum^q \tau(R_i) \geq \tau_{LP}(p, q),$$

Proof. Set

$$(d_i^0, t_i^0) = (\text{dih}(S_i), \tau(S_i)), \quad (d_i^1, t_i^1) = (\text{dih}(R_i), \tau(R_i)).$$

Then $\sum^p \tau(S_i) + \sum^q \tau(R_i)$ is at least the minimum of $\sum^p t_i^0 + \sum^q t_i^1$ subject to $\sum^p d_i^0 + \sum^q d_i^1 = 2\pi$ and to the system of linear inequalities of Section 10 (Group 3) and Proposition 4.1 (obtained by replacing $-\sigma_1$ and dihedral angles by t_i^j and d_i^j). The constant $\tau_{LP}(p, q)$ was chosen to be slightly larger than the actual minimum of this linear programming problem.

The entry $\tau_{LP}(5, 0)$ is based on Lemma 5.3, $k = 1$. \square

Lemma 5.3. *Let v_1, \dots, v_k , for some $k \leq 4$, be distinct vertices of a decomposition star of type $(5, 0)$. Let S_1, \dots, S_r be quasi-regular tetrahedra around the edges $(0, v_i)$, for $i \leq k$. Then*

$$\sum_{i=1}^r \tau(S_i) > 0.55k pt,$$

and

$$\sum_{i=1}^r \sigma(S_i) < r pt - 0.48k pt.$$

Proof. We have $\tau(S) \geq 0$, for any quasi-regular tetrahedron S . We refer to the edges y_4, y_5, y_6 of a simplex $S(y_1, \dots, y_6)$ as its top edges. Set $\xi = 2.1773$.

We claim (Claim 1) that if S_1, \dots, S_5 are quasi-regular tetrahedra around an edge $(0, v)$ and if $S_1 = S(y_1, \dots, y_6)$, where $y_5 \geq \xi$ is the length of a top edge e on S_1 shared with S_2 , then $\sum_1^5 \tau(S_i) > 3(0.55)pt$. This claim follows from Inequalities 10.5.1 and 10.5.2 if some other top edge in this group of quasi-regular tetrahedra has length greater than ξ . Assuming all the top edges other than e have length at most ξ , the estimate follows from $\sum_1^5 \text{dih}(S_i) = 2\pi$ and Inequalities 10.5.3, 10.5.4.

Now let S_1, \dots, S_8 be the eight quasi-regular tetrahedra around two edges $(0, v_1), (0, v_2)$ of type $(5, 0)$. Let S_1 and S_2 be the simplices along the face $(0, v_1, v_2)$. Suppose that the top edge (v_1, v_2) has length at least ξ . We claim (Claim 2) that $\sum_1^8 \tau(S_i) > 4(0.55)pt$. If there is a top edge of length at least ξ that does not lie on S_1 or S_2 , then this claim reduces to Inequality 10.5.1 and Claim 1. If any of the top edges of S_1 or S_2 other than (v_1, v_2) has length at least ξ , then the claim follows from Inequalities 10.5.1 and 10.5.2. We assume all top edges other than (v_1, v_2) have length at most ξ . The claim now follows from Inequalities 10.5.3 and 10.5.5, since the dihedral angles around each vertex sum to 2π .

We prove the bounds for τ . The proof for σ is entirely similar, but uses the constant $\xi = 2.177303$ and the Inequalities 10.5.8–10.5.14 rather than 10.5.1–10.5.7. Claims analogous to Claims 1 and 2 hold for the σ bound by Inequalities 10.5.8–10.5.12.

Consider τ for $k = 1$. If a top edge has length at least ξ , this is Inequality 10.5.1. If all top edges have length less than ξ , this is Inequality 10.5.3, since dihedral angles sum to 2π .

We say that a top edge lies around a vertex v if it is an edge of a quasi-regular tetrahedron with vertex v . We do not require v to be the endpoint of the edge.

Take $k = 2$. If there is an edge of length at least ξ that lies around only one of v_1 and v_2 , then Inequality 10.5.1 reduces us to the case $k = 1$. Any other edge of length at least ξ is covered by Claim 1. So we may assume that all top edges have length less than ξ . And then the result follows easily from Inequalities 10.5.3 and 10.5.6.

Take $k = 3$. If there is an edge of length at least ξ lying around only one of the v_i , then Inequality 10.5.1 reduces us to the case $k = 2$. If an edge of length at least ξ lies around exactly two of the v_i , then it is an edge of two of the quasi-regular tetrahedra. These quasi-regular tetrahedra give $2(0.55)pt$, and the quasi-regular tetrahedra around the third vertex v_i give $0.55pt$ more. If a top edge of length at least ξ lies around all three vertices, then one of the endpoints of the edge lies in $\{v_1, v_2, v_3\}$, so the result follows from Claim 1. Finally, if all top edges have length at most ξ , we use Inequalities 10.5.3, 10.5.6, 10.5.7.

Take $k = 4$. Suppose there is a top edge e of length at least ξ . If e lies around only one of the v_i , we reduce to the case $k = 3$. If it lies around two of them, then the two quasi-regular tetrahedra along this edge give $2(0.55)pt$ and the quasi-regular tetrahedra around the other two vertices v_i give another $2(0.55)pt$. If both endpoints of e are among the vertices v_i , the result follows from Claim 2. This happens in particular if e lies around four vertices. If e lies around only three

vertices, one of its endpoints is one of the vertices v_i , say v_1 . Assume e is not around v_2 . If v_2 is not adjacent to v_1 , then Claim 1 gives the result. So taking v_1 adjacent to v_2 , we adapt Claim 1, by using Inequalities 10.5.1–10.5.7, to show that the eight quasi-regular tetrahedra around v_1 and v_2 give $4(0.55)pt$. Finally, if all top edges have length at most ξ , we use Inequalities 10.5.3, 10.5.6, 10.5.7. \square

6. LIMITATIONS ON TYPES

Recall that a vertex of a planar map has type (p, q) if it is the vertex of exactly p triangles and q quadrilaterals. This section restricts the possible types that appear in a decomposition star.

Let t_4 denote the constant $0.1317 \approx 2.37838774pt$. Proposition 4.1.11 asserts that every quad cluster R satisfies $\tau(R) \geq t_4$.

Lemma 6.1. *The following eight types (p, q) are impossible: (1) $p \geq 8$, (2) $p \geq 6$ and $q \geq 1$, (3) $p \geq 5$ and $q \geq 2$, (4) $p \geq 4$ and $q \geq 3$, (5) $p \geq 2$ and $q \geq 4$, (6) $p \geq 0$ and $q \geq 6$, (7) $p \leq 3$ and $q = 0$, (8) $p \leq 1$ and $q = 1$.*

Proof. By Proposition 4.1.3 and Calculation 10.1.3, a lower bound on the dihedral angle of p simplices and q quadrilaterals is $0.8638p + 1.153q$. If the type exists, this constant must be at most 2π . One readily verifies in Cases 1–6 that $0.8638p + 1.153q > 2\pi$. By Proposition 4.3 and Calculation 10.1.2, an upper bound on the dihedral angle of p triangles and q quadrilaterals is $1.874445p + 3.247q$. In Cases 7 and 8 this constant is less than 2π . \square

Lemma 6.2. *If the type of any vertex of a decomposition star is one of $(4, 2)$, $(3, 3)$, $(1, 4)$, $(1, 5)$, $(0, 5)$, $(0, 2)$, $(7, 0)$, then the decomposition star scores less than $8pt$.*

Proof. According to Table 5.1, we have $\tau_{LP}(p, q) > (4\pi\zeta - 8)pt$, for $(p, q) = (4, 2)$, $(3, 3)$, $(1, 4)$, $(1, 5)$, $(0, 5)$, or $(0, 2)$. By Lemma 3.2, the result follows in these cases. Now suppose that one of the vertices has type $(7, 0)$. By the results of Part I, which treats the case in which all standard regions are triangles, we may assume that the star has at least one quadrilateral. We then have $\tau(D^*) \geq \tau_{LP}(7, 0) + t_4 > (4\pi\zeta - 8)pt$. The result follows. \square

In summary of the preceding two lemmas, we find that we may restrict our attention to the following types of vertices.

$$\begin{array}{rcl}
 (6, 0) & & \\
 (5, 0) & (5, 1) & \\
 (4, 0) & (4, 1) & \\
 & (3, 1) & (3, 2) \\
 & (2, 1) & (2, 2) \quad (2, 3) \\
 & & (1, 2) \quad (1, 3) \\
 & & (0, 3) \quad (0, 4)
 \end{array}$$

7. PROPERTIES OF PLANAR MAPS

Proposition 7.1. *Suppose that $\sigma(D^*) \geq 8pt$. The planar map L of D^* has the following properties (without loss of generality):*

1. The graph $G(L)$ has no loops or multiple joins.
2. Each face of L is a triangle or quadrilateral.
3. L has at least eight triangular faces.
4. L has at most six quadrilateral faces, and at least one.
5. Each vertex has one of the following types: $(6, 0)$, $(5, 0)$, $(4, 0)$, $(5, 1)$, $(4, 1)$, $(3, 1)$, $(2, 1)$, $(3, 2)$, $(2, 2)$, $(1, 2)$, $(2, 3)$, $(1, 3)$, $(0, 3)$, and $(0, 4)$.
6. If C is a 3-circuit in $G(L)$, then it bounds a triangular face.
7. If C is a 4-circuit in $G(L)$, then one of the following is true:
 - (a) C bounds some quadrilateral region,
 - (b) C bounds a pair of adjacent triangles,
 - (c) C encloses one vertex, and it has type $(4, 0)$ or $(2, 1)$.
8. $t_4q + \sum_{v \in V} (\tau_{LP}(p_v, q_v) - t_4q_v) \leq (4\pi\zeta - 8)pt$, for any collection V of vertices in L such that no two vertices of V lie on a common face.

Proof. A loop would give a closed geodesic on the unit sphere of length less than π . A multiple join would give nonantipodal conjugate points on the sphere. Property 2 is the restriction of step 3 of the Kepler conjecture. Property 3 follows from I.9.1 and Part II. Property 4 follows from $7t_4 > (4\pi\zeta - 8)pt$. If there are no quadrilaterals, the problem has been solved in Part I. The restrictions on types were obtained in Section 6. Property 6 is established in Part I. A 4-circuit encloses at most one vertex by I.4.2. If it encloses none, it gives a quad cluster or two tetrahedra. Otherwise, it encloses a vertex of type $(4, 0)$ or type $(2, 1)$. Property 8 comes from Section 5. \square

8. COMBINATORICS

In Steps III and IV of the Kepler conjecture, we need to generate all planar maps satisfying various lists of conditions. Here we describe a computer algorithm, which has been implemented in *Java*. We describe the algorithm in a way that it can be used for Step IV as well.

We assume that the planar maps satisfy the following conditions.

1. There are no loops or multiple joins.
2. Each face is a polygon.
3. The graph has between 3 and N vertices, for some explicit N .
4. The degree at each vertex is at most 6.
5. If C is a 3-circuit in $G(L)$, then C bounds a triangular face.

6. If C is a 4-circuit in $G(L)$, then one side of C contains at most 1 vertex.
7. There is a constant $T \geq 0$ and constants $t_n \geq 0$ and $t(p, q, r) \geq 0$, such that

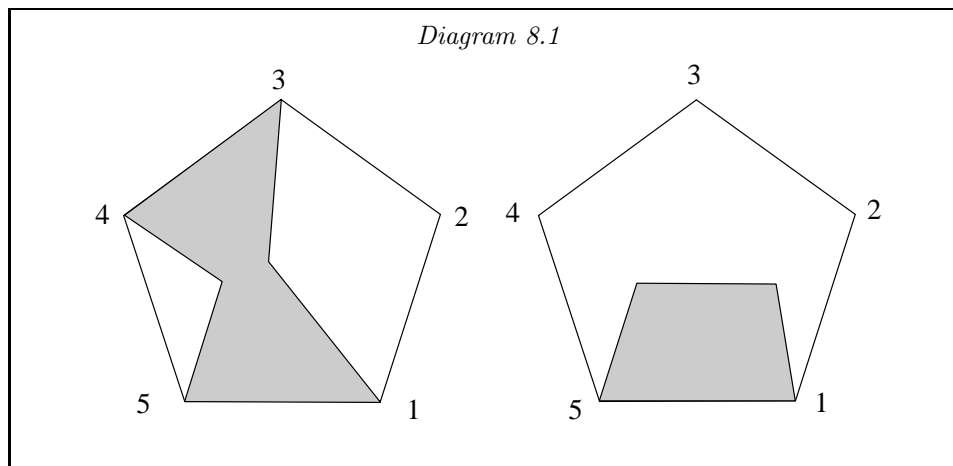
$$\sum_I t_n + \sum_V \tau_{\text{LP}}(p_v, q_v, r_v) < T,$$

where the first sum runs over *finished* faces, and the second sum runs over any *separated* set of vertices. (The term *finished* will be described below. For planar maps produced as output of the algorithm, every face will be finished. But at intermediate stages of the algorithm some will be unfinished.) Also, a separated set of vertices means a collection of vertices with the properties that no two lie on a common face, and that every face at each of the vertices is finished. Here p_v is the number of triangles, q_v is the number of quadrilaterals, r_v is the number of other regions at v , and $n = n_v = p_v + q_v + r_v$. Also, n is the number of sides of the finished face.

There are additional properties that it might be helpful to impose, but the ones stated are sufficient for the description of the algorithm. In our context, $r = r_v = 0$, $t_3 = 0$, $T = (4\pi\zeta - 8)pt$, $t_4 = 0.1317$ and $t(p, q, 0) = \tau_{\text{LP}}(p, q) - t_4q$.

We produce all maps satisfying the conditions 1–7, by extending maps already satisfying these properties. We assume that we have a stack of maps $\{L_j : j \in J\}$ satisfying the conditions 1–7 such that each face of each of these maps is labeled finished or unfinished. Each planar map in the stack will have at least one unfinished face. In one iteration of the algorithm, we pop one of the maps L from the stack, modify it in various ways to produce new maps, output any of the new maps that are finished (meaning all faces are finished), and push the remaining ones back on the stack. When all maps have been popped from the stack, we are guaranteed to have produced all finished maps satisfying properties (1–7). Here are the details of the algorithm.

1. Let L be a planar map that has been popped from the stack. Fix any unfinished face F of L and any edge e of F . Label the vertices of F consecutively $1, \dots, \ell$, with 1 and ℓ the endpoints of e . For each $m = 3, \dots, N$, let A_m be the set of all m -tuples $(a_i) \in \mathbb{Z}^m$ satisfying $(1 = a_1 \leq a_2 \leq \dots \leq a_m = \ell)$, with $a_{m-1} \neq a_m$.
2. For each $a \in A_m$, we draw a new m -gon F_a along the edge e of F as follows. We construct the vertices $v(1), \dots, v(m)$ inductively. If $i = 1$ or $a_i \neq a_{i-1}$, then we set $v(i) = \text{vertex } a_i \text{ of } F$. But if $a_i = a_{i-1}$, we add a new vertex $v(i)$ to the planar map. The new face is to be drawn along the edge e over the face F . (For example, when $\ell = 5$, the faces F_a corresponding to $a = (1, 1, 3, 4, 4, 5)$ and $a = (1, 1, 1, 5)$ are shown in Diagram 8.1.) As we run over all m and $a \in A_m$, we run over all possibilities for the finished face along the edge e inside F .



3. The face F_a is to be marked as finished. By drawing F_a , F is broken into a number of smaller polygons. (In Diagram 8.1, F is replaced respectively by three and two polygons.) Each of these smaller polygons other than F_a is taken to be unfinished, except triangles, which are always taken to be finished.

4. Various planar maps extending L are obtained by this process. Those that do not satisfy the conditions (1–7) are discarded. Those that have no unfinished faces are output. The remaining ones are pushed back onto the stack. If the stack is empty, the program terminates. Otherwise, we pop a planar map from the stack and return to the first step. It is condition 7 that forces the algorithm to terminate.

To begin the algorithm, we need an initial stack of planar maps. The planar maps in the initial stack will be called *seeds*. To produce a list of seeds, it is enough to give any list that is guaranteed to produce all possibilities by the algorithm described in 1, \dots , 4. For example, for Part III we want all configurations with at least one quadrilateral and nothing but triangles and quadrilaterals. We could let our initial stack consist of a single planar map L , where the graph $G(L)$ is a single 4-cycle. Also, L is to have two faces, a finished quadrilateral and an unfinished complement. Then by iterating through the steps 1, \dots , 4, we generate all possible extensions of a quadrilateral to a planar map satisfying 1, \dots , 7.

Although this seed would work, in order to improve the performance of the algorithm, in the implementation used for this paper, we used a more detailed list of seeds, based on the classification of types (p, q) in Section 6.

This algorithm produced 1762 cases, even when the additional properties listed in Proposition 7.1 were used. To be exact, a few of the maps may be superfluous, because there was no need to discard every last map that we were allowed to. The important point is that an explicit finite list was obtained. Because of the number of possibilities involved we have not listed them here. The Java source code and pictures of the maps are available at [H2].

9. LINEAR PROGRAMMING BOUNDS

For each of the planar maps produced in Section 8, we define a linear programming

problem whose solution dominates the score of the decomposition stars associated with the planar map. A description of the linear programs is presented in this section.

Theorem 9.1. *Let L be any planar map obtained in Section 8. One of the following holds. (1) L is the planar map of the pentagonal prism, hexagonal-close packing, or face-centered cubic. (2) Every decomposition star with planar map L scores less than $8pt$. (3) L is one of the 18 cases presented in Appendix I.*

The variables of the linear programming problem are the dihedral angles, the scores of each of the standard clusters, and their edge lengths.

We subject these variables to a system of linear inequalities. First of all, the dihedral angles around each vertex sum to 2π . The dihedral angles, solid angles, and score are related by the linear inequalities of Groups 1, 2, 3, and 4 in Section 10. These include Propositions 4.1 and 4.2. The solid-angle variables are linear functions of dihedral angles. The score of a decomposition star is

$$\sigma(S_1) + \cdots + \sigma(S_p) + \sigma(R_1) + \cdots + \sigma(R_q).$$

Forgetting the origin of the scores, solid angles, and dihedral angles as nonlinear functions of the standard clusters and treating them as formal variables subject only to the given linear inequalities, we obtain a linear programming bound on the score.

Floating-point arithmetic was used freely in obtaining these bounds. The linear programming package *CPLEX* was used (see www.cplex.com). However, the results, once obtained, could be checked rigorously as follows. (We did not actually do this because the precision never seemed to be an issue, but this is how it can easily be done.¹) For each quasi-regular tetrahedron S_i we have a nonnegative variable $x_i = pt - \sigma(S_i)$. For each quad cluster R_k , we have a nonnegative variable $x_k = -\sigma(R_k)$. A bound on the score is $ppt - \sum_{i \in I} x_i$, where p is the number of triangular standard regions, and I indexes the faces of the planar map. We give error bounds for a linear program involving scores and dihedral angles. Similar estimates can be made if there are edges representing edge lengths. Let the dihedral angles be x_j , for j in some indexing set J . Write the linear constraints as $Ax \leq b$. We wish to maximize $c \cdot x$ subject to these constraints, where $c_i = -1$, for $i \in I$, and $c_j = 0$, for $j \in J$. Let z be an approximate solution to the inequalities $zA \geq c$ and $z \geq 0$ obtained by numerical methods. Replacing the negative entries of z by 0 we may assume that $z \geq 0$ and that $zA_i > c_i - \epsilon$, for $i \in I \cup J$, and some small error ϵ . If we obtain the numerical bound $ppt + z \cdot b < 7.9999pt$, and if $\epsilon < 10^{-8}$, then the score is less than $8pt$. In fact, note that

$$\left(\frac{z}{1 + \epsilon} \right) A_i$$

is at least c_i for $i \in I$ (since $c_i = -1$), and that it is greater than $c_i - \epsilon/(1 + \epsilon)$, for $i \in J$ (since $c_i = 0$). Thus, if $N \leq 60$ is the number of vertices, and $p \leq 2(N - 2) \leq$

¹The output from each linear program in this paper has been double checked with interval arithmetic. Predictably, the error bounds presented here were satisfactory. 1/2002

116 is the number of triangular faces,

$$\begin{aligned}
\sigma(D^*) &\leq p \, pt + c \cdot x \leq p \, pt + \left(\frac{z}{1+\epsilon} \right) Ax + \frac{\epsilon}{1+\epsilon} \sum_{j \in J} x_j \\
&\leq p \, pt + \frac{z \cdot b}{1+\epsilon} + \frac{\epsilon}{1+\epsilon} 2\pi N \\
&\leq [p \, pt + z \cdot b + \epsilon(p \, pt + 2\pi N)] / (1+\epsilon) \\
&\leq [7.9999 \, pt + 10^{-8}(116 \, pt + 500)] / (1+10^{-8}) < 8 \, pt.
\end{aligned}$$

In practice, we used $0.4429 < 0.79984 \, pt$ as our cutoff, and $N \leq 14$ in the interesting cases, so much tighter error estimates are possible.

10. CALCULATIONS

In each of these calculations, when the cluster is a quasi-regular tetrahedron S , we set $\sigma = \sigma(S)$, $\text{dih} = \text{dih}(S)$, and so forth. Let $\sigma_\lambda = \sigma - \lambda \zeta \, pt \, \text{sol}$, for $\lambda = 1, 3, 2$. We make similar abbreviations for quad clusters. The inequalities in Group 1 follow from results appearing elsewhere. These inequalities have been verified by interval arithmetic in [H2].

Group 1. Calculations that have been verified elsewhere.

Quasi-regular tetrahedra:

1. $\sigma \leq pt$ (I.9.1),
2. $\text{dih} < 1.874445$ (I.8.3.2),
3. $\text{dih} > 0.8638$ (I.9.3),
4. $\sigma < -0.37642101 \, \text{sol} + 0.287389$ (I.9.8),
5. $\sigma < 0.446634 \, \text{sol} - 0.190249$ (I.9.9),
6. $\sigma < -0.419351 \, \text{sol} + 0.2856354 + 0.001$ (I.9.10, I.9.11, I.9.12, I.9.18).

Quad clusters:

7. $\sigma \leq 0$ (II).

Group 2. Inequalities for quasi-regular tetrahedra depending on edge lengths.

1. $\text{sol} > 0.551285 + 0.199235(y_4 + y_5 + y_6 - 6) - 0.377076(y_1 + y_2 + y_3 - 6)$,
2. $\text{sol} < 0.551286 + 0.320937(y_4 + y_5 + y_6 - 6) - 0.152679(y_1 + y_2 + y_3 - 6)$,
3. $\text{dih} > 1.23095 - 0.359894(y_2 + y_3 + y_5 + y_6 - 8) + 0.003(y_1 - 2) + 0.685(y_4 - 2)$,
4. $\text{dih} < 1.23096 - 0.153598(y_2 + y_3 + y_5 + y_6 - 8) + 0.498(y_1 - 2) + 0.76446(y_4 - 2)$,
5. $\sigma < 0.0553737 - 0.10857(y_1 + \dots + y_6 - 12)$,
6. $\sigma + 0.419351 \, \text{sol} < 0.28665 - 0.2(y_1 + y_2 + y_3 - 6)$,
7. $\sigma_1 < 10^{-6} - 0.129119(y_4 + y_5 + y_6 - 6) - 0.0845696(y_1 + y_2 + y_3 - 6)$.

Group 3. General inequalities for quad clusters and quasi-regular tetrahedra.

Quasi-regular tetrahedra:

1. $\sigma < 0.37898 \, \text{dih} - 0.4111$,
2. $\sigma < -0.142 \, \text{dih} + 0.23021$,
3. $\sigma < -0.3302 \, \text{dih} + 0.5353$,
4. $\sigma_1 < 0.3897 \, \text{dih} - 0.4666$,

5. $\sigma_1 < 0.2993 \text{ dih} - 0.3683$,
6. $\sigma_1 \leq 0$,
7. $\sigma_1 < -0.1689 \text{ dih} + 0.208$,
8. $\sigma_1 < -0.2529 \text{ dih} + 0.3442$,
9. $\sigma_{3.2} < 0.4233 \text{ dih} - 0.5974$,
10. $\sigma_{3.2} < 0.1083 \text{ dih} - 0.255$,
11. $\sigma_{3.2} < -0.0953 \text{ dih} - 0.0045$,
12. $\sigma_{3.2} < -0.1966 \text{ dih} + 0.1369$,
13. $\sigma < -0.419351 \text{ sol} + 0.796456 \text{ dih} - 0.5786316$,
14. $\sigma < -0.419351 \text{ sol} + 0.0610397 \text{ dih} + 0.211419$,
15. $\sigma < -0.419351 \text{ sol} - 0.0162028 \text{ dih} + 0.308526$,
16. $\sigma < -0.419351 \text{ sol} - 0.0499559 \text{ dih} + 0.35641$,
17. $\sigma < -0.419351 \text{ sol} - 0.64713719 \text{ dih} + 1.3225$.

Quad clusters: Propositions 4.1 and 4.2.

Group 4. Miscellaneous inequalities.

Quasi-regular tetrahedra:

1. The quasi-regular tetrahedra at a vertex of type $(4, 0)$ score at most 0.33 pt (I.5.2).
2. The sum of the dihedral angles around a vertex is 2π .
3. The five quasi-regular tetrahedra S_i at a vertex of type $(5, 0)$ satisfy

$$\sum \sigma(S_i) < \sum (-0.419351 \text{ sol}(S_i) + 0.2856354)$$

(I.5.1.1).

Flat quarters:

4. $-0.398(y_2 + y_3 + y_5 + y_6) + 0.3257y_1 - \text{dih}_1 < -4.14938$,
if $y_4 \geq 2.51$.
5. Proposition 4.3, Lemma 5.3.
6. Inequalities of Appendix 1: A.2.1–11, A.3.1–11, A.4.1–4, A.6.1–9, A.6.1'–8', A.8.1–3.

Group 5. Inequalities used by Lemma 5.3.

quasi-regular tetrahedra: Let $\xi = 2.1773$, $m = 0.2384$.

1. If $y_4 \geq \xi$, then $\tau > 0.55 \text{ pt}$,
2. If $y_4, y_5 \geq \xi$, then $\tau > 2(0.55) \text{ pt}$,
3. If $y_4 \leq \xi$, then $\tau > -0.29349 + m \text{ dih}$,
4. If $y_4, y_6 \leq \xi$, $y_5 \geq \xi$, then $\tau > -0.26303 + m \text{ dih}$,
5. If $y_6 \geq \xi$, $y_4, y_5 \leq \xi$, then $\tau > -0.5565 + m(\text{dih}_1 + \text{dih}_2)$,
6. If $y_4, y_5, y_6 \leq \xi$, then $\tau > -2(0.29349) + m(\text{dih}_1 + \text{dih}_2)$,
7. If $y_4, y_5, y_6 \leq \xi$, then $\tau > -3(0.29349) + m(\text{dih}_1 + \text{dih}_2 + \text{dih}_3)$.

Now set $\xi = 2.177303$, $m = 0.207045$.

8. If $y_4 \geq \xi$, then $\sigma < (1 - 0.48) \text{ pt}$,
9. If $y_4, y_5 \geq \xi$, then $\sigma < (1 - 2(0.48)) \text{ pt}$,
10. If $y_4 \leq \xi$, then $\sigma < 0.31023815 - m \text{ dih}$,
11. If $y_4, y_6 \leq \xi$, $y_5 \geq \xi$, then $\sigma < 0.28365 - m \text{ dih}$,
12. If $y_6 \geq \xi$, $y_4, y_5 \leq \xi$, then $\sigma < 0.53852 - m(\text{dih}_1 + \text{dih}_2)$,
13. If $y_4, y_5, y_6 \leq \xi$, then $\sigma < -\text{pt} + 2(0.31023815) - m(\text{dih}_1 + \text{dih}_2)$,
14. If $y_4, y_5, y_6 \leq \xi$, then $\sigma < -2 \text{ pt} + 3(0.31023815) - m(\text{dih}_1 + \text{dih}_2 + \text{dih}_3)$.

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APPENDIX 1. SOME FINAL CASES

The graphs are numbered in the archive from 0 to 1761. There are three cases that are treated elsewhere: PM(4, 1679) is the face-centered cubic, PM(4, 1672) is the pentahedral prism, and PM(4, 1640) is the hexagonal close packing.

The body of this paper eliminates all but a couple of dozen planar maps. (The explicit list appears in the archive [H2].) This appendix indicates how to eliminate the final cases. The archive contains a few graphs that are isomorphic to each other. The following discussion assumes that these duplicates have been eliminated. To exploit the nonlinearities of the problem, we use a branch-and-bound method and divide the domains of the optimization problem into several thousand smaller sets. A linear programming bound of 8 *pt* is obtained in each case. This appendix lists all of the inequalities that have been used, and gives a description of the cases. We refer the reader to [H2] for details about computer implementation of the linear programs.

A.1. Types. Each quad cluster with corners (v_1, v_2, v_3, v_4) is one of four types [F]. Although it was advantageous to group these cases together to simplify the combinatorics, it is now better to separate these cases and to develop linear inequalities for each case.

1. Two flat quarters with diagonal (v_1, v_3) . The score of each quarter is compression or the analytic Voronoi function.
2. Two flat quarters with diagonal (v_2, v_4) . The score of each quarter is compression or the analytic Voronoi function.
3. Four upright quarters forming an octahedron. The score of each upright quarter is compression or the averaged analytic Voronoi function $\text{octavor}(Q) = (\text{vor}(Q) + \text{vor}(\hat{Q}))/2$. In other words, $\sigma(Q) = (\mu(Q) + \mu(\hat{Q}))/2$. We are using notation from [F].
4. One of various mixed quad clusters. The score is at most vor_0 , the truncated Voronoi function at radius $t_0 = 1.255$.

A.2. Flat quarters. For flat quarters, we have the following inequalities that were established by interval arithmetic. The edge y_4 is taken to be the diagonal of the flat quarter. Here $\sigma = \mu$.

1. $-\text{dih}_2 + 0.35y_2 - 0.15y_1 - 0.15y_3 + 0.7022y_5 - 0.17y_4 > -0.0123$,
2. $-\text{dih}_3 + 0.35y_3 - 0.15y_1 - 0.15y_2 + 0.7022y_6 - 0.17y_4 > -0.0123$,
3. $\text{dih}_2 - 0.13y_2 + 0.631y_1 + 0.31y_3 - 0.58y_5 + 0.413y_4 + 0.025y_6 > 2.63363$,
4. $\text{dih}_3 - 0.13y_3 + 0.631y_1 + 0.31y_2 - 0.58y_6 + 0.413y_4 + 0.025y_5 > 2.63363$,
5. $-\text{dih}_1 + 0.714y_1 - 0.221y_2 - 0.221y_3 + 0.92y_4 - 0.221y_5 - 0.221y_6 > 0.3482$,
6. $\text{dih}_1 - 0.315y_1 + 0.3972y_2 + 0.3972y_3 - 0.715y_4 + 0.3972y_5 + 0.3972y_6 > 2.37095$,
7. $-\text{sol} - 0.187y_1 - 0.187y_2 - 0.187y_3 + 0.1185y_4 + 0.479y_5 + 0.479y_6 > 0.437235$,
8. $\text{sol} + 0.488y_1 + 0.488y_2 + 0.488y_3 - 0.334y_5 - 0.334y_6 > 2.244$,
9. $-\sigma - 0.159y_1 - 0.081y_2 - 0.081y_3 - 0.133y_5 - 0.133y_6 > -1.17401$,
10. $\sigma < -0.419351\text{sol} + 0.1448 + 0.0436(y_5 + y_6 - 4) + 0.079431\text{dih}$,
11. $\sigma < 10^{-6} - 0.197(y_4 + y_5 + y_6 - 2\sqrt{2} - 4)$.

A.3. Upright quarters. The following inequalities for upright quarters have been established by interval arithmetic. The first edge is taken to be the upright

diagonal.

1. $\text{dih}_1 - 0.636y_1 + 0.462y_2 + 0.462y_3 - 0.82y_4 + 0.462y_5 + 0.462y_6 > 1.82419$,
2. $-\text{dih}_1 + 0.55y_1 - 0.214y_2 - 0.214y_3 + 1.24y_4 - 0.214y_5 - 0.214y_6 > 0.75281$,
3. $\text{dih}_2 + 0.4y_1 - 0.15y_2 + 0.09y_3 + 0.631y_4 - 0.57y_5 + 0.23y_6 > 2.5481$,
4. $-\text{dih}_2 - 0.454y_1 + 0.34y_2 + 0.154y_3 - 0.346y_4 + 0.805y_5 > -0.3429$,
5. $\text{dih}_3 + 0.4y_1 - 0.15y_3 + 0.09y_2 + 0.631y_4 - 0.57y_6 + 0.23y_5 > 2.5481$,
6. $-\text{dih}_3 - 0.454y_1 + 0.34y_3 + 0.154y_2 - 0.346y_4 + 0.805y_6 > -0.3429$,
7. $\text{sol} + 0.065y_2 + 0.065y_3 + 0.061y_4 - 0.115y_5 - 0.115y_6 > 0.2618$,
8. $-\text{sol} - 0.293y_1 - 0.03y_2 - 0.03y_3 + 0.12y_4 + 0.325y_5 + 0.325y_6 > 0.2514$,
9. $-\sigma - 0.054y_2 - 0.054y_3 - 0.083y_4 - 0.054y_5 - 0.054y_6 > -0.59834$,
10. $\sigma < -0.419351 \text{ sol} + 0.079431 \text{ dih}_2 + 0.06904 - 0.0846(y_1 - 2.8)$,
11. If $y_2, y_3 \leq 2.13$, then $\sigma < 0.07(y_1 - 2.51) - 0.133(y_2 + y_3 + y_5 + y_6 - 8) - 0.135(y_4 - 2)$.

A.4. Truncated quad clusters. Let $\phi(h, t) = (4 - 2\delta_{\text{oct}}ht(h + t))/3$. Set $t_0 = 1.255$ and $\phi_0 = \phi(t_0, t_0)$. In the truncated case vor_0 , [F] gives

$$\text{vor}_0 = \phi_0 \text{ sol} + \sum A(y_i/2) \text{ dih}_i - 4\delta_{\text{oct}} \sum_R \text{quo}(R),$$

with $\phi_0 = \phi(t_0, t_0)$, and

$$A(h) = (1 - h/t_0)(\phi(h, t_0) - \phi(t_0, t_0)).$$

Let R be the Rogers simplex $R(y_1/2, \eta(y_1, y_2, y_6), t_0)$. The function $\text{quo}(R)$ is defined in [F.3.3]. We have $\text{quo}(R) \geq 0$. Let vor_0^A denote the truncated Voronoi score of half the quad cluster, divided into two simplices along a diagonal, obtained by applying the formula for vor_0 to the simplex. The following inequalities hold by interval arithmetic:

1. $\text{dih} - 0.372y_1 + 0.465y_2 + 0.465y_3 + 0.465y_5 + 0.465y_6 > 4.885$,
 2. $-\text{vor}_0^A - 0.06y_2 - 0.06y_3 - 0.185y_5 - 0.185y_6 > -0.9978$,
- provided $\text{dih} < 2.12$, and $y_1, y_2, y_3 \leq 2.26$,
3. $-\text{vor}_0^A + 0.419351 \text{ sol}^A < 0.3072$,
- provided $\text{dih} < 2.12$, and $y_1, y_2, y_3 \leq 2.26$,
4. $\text{quo} + 0.00758y_1 + 0.0115y_2 + 0.0115y_6 > 0.06333$.

Also, $A \geq 0$, $A' \leq 0$, and $A'' \geq 0$, for $h \in [1, t_0]$. If $\text{dih} \in [\text{dih}_{\min}, \text{dih}_{\max}]$, and $h \in [1, h_{\max}]$, for some constants dih_{\min} , dih_{\max} , and $1 < h_{\max} \leq t_0$, then setting $\lambda = (A(h_{\max}) - A(1))/(h_{\max} - 1)$, we obtain the additional elementary inequalities for $Ad := A(h) \text{ dih}$.

5. $Ad - A(1) \text{ dih} \leq \lambda(h - 1) \text{ dih}_{\min}$,
6. $Ad \leq (A(1) + \lambda(h - 1)) \text{ dih}_{\max}$.

We use linear programming methods to determine bounds h_{\max} , dih_{\min} , dih_{\max} . If $Ax \leq b$ is the system of inequalities used in the linear programs in the main body of the paper, then we obtain an upper bound on a variable y by solving the linear program $\max y$ subject to the constraints $Ax \leq b$, and the constraint that the sum of the variables σ (that is, the linear variables corresponding to the score) is at least $8pt$.

A.5. Linear programs.

Consider one of the remaining cases $PM = PM(4, n)$. Suppose PM has r quadrilateral faces. We run 4^r linear programs, depending on which type 1–4 of quad cluster from A.1 each quadrilateral face represents. In each case, we add the additional linear inequalities from A.2, A.3, or A.4 as appropriate. Note that a few of these inequalities are only conditionally true, so that the inequality can be used only if it is known that the condition holds. All of the planar maps have bounds under 8 *pt* by this method, except for $PM(4, 71)$, $PM(4, 118)$, $PM(4, 126)$, and $PM(4, 178)$.

A.6. Quasi-regular tetrahedra.

The first nine inequalities assume that $y_4 + y_5 + y_6 \leq 6.25$. Of these, the last two are established only under the additional assumptions $y_1, y_2, y_3 \leq 2.13$. The next eight inequalities assume that $y_4 + y_5 + y_6 \geq 6.25$. Of these, the last three assume that $y_1, y_2, y_3 \leq 2.13$.

1. $\text{sol} + 0.377076y_1 + 0.377076y_2 + 0.377076y_3 - 0.221y_4 - 0.221y_5 - 0.221y_6 > 1.487741,$
2. $0.221y_4 + 0.221y_5 + 0.221y_6 - \text{sol} > 0.76822,$
3. $\text{dih} + 0.34y_2 + 0.34y_3 - 0.689y_4 + 0.27y_5 + 0.27y_6 > 2.29295,$
4. $-\text{dih} + 0.498y_1 + 0.731y_4 - 0.212y_5 - 0.212y_6 > 0.37884,$
5. $-\sigma - 0.109y_1 - 0.109y_2 - 0.109y_3 - 0.14135y_4 - 0.14135y_5 - 0.14135y_6 > -1.5574737,$
6. $-\sigma - 0.419351\text{sol} - 0.2y_1 - 0.2y_2 - 0.2y_3 - 0.048y_4 - 0.048y_5 - 0.048y_6 > -1.77465,$
7. $\tau - 0.0845696y_1 - 0.0845696y_2 - 0.0845696y_3 - 0.163y_4 - 0.163y_5 - 0.163y_6 > -1.48542,$
8. $\text{dih} + 0.27y_2 + 0.27y_3 - 0.689y_4 + 0.27y_5 + 0.27y_6 > 2.01295, \text{ if } y_1, y_2, y_3 \leq 2.13.$
9. $-\sigma - 0.14135y_1 - 0.14135y_2 - 0.14135y_3 - 0.14135y_4 - 0.14135y_5 - 0.14135y_6 > -1.7515737, \text{ if } y_1, y_2, y_3 \leq 2.13.$

- 1'. $y_4 + y_5 + y_6 > 6.25,$
- 2'. $\text{sol} + 0.378y_1 + 0.378y_2 + 0.378y_3 - 0.1781y_4 - 0.1781y_5 - 0.1781y_6 > 1.761445,$
- 3'. $-\text{sol} - 0.171y_1 - 0.171y_2 - 0.171y_3 + 0.3405y_4 + 0.3405y_5 + 0.3405y_6 > 0.489145,$
- 4'. $-\sigma - 0.1208y_1 - 0.1208y_2 - 0.1208y_3 - 0.0781y_4 - 0.0781y_5 - 0.0781y_6 > -1.2436,$
- 5'. $-\sigma - 0.419351\text{sol} - 0.2y_1 - 0.2y_2 - 0.2y_3 + 0.0106y_4 + 0.0106y_5 + 0.0106y_6 > -1.40816,$
- 6'. $\text{sol} + 0.356y_1 + 0.356y_2 + 0.356y_3 - 0.1781y_4 - 0.1781y_5 - 0.1781y_6 > 1.629445,$
if $y_1, y_2, y_3 \leq 2.13,$
- 7'. $-\text{sol} - 0.254y_1 - 0.254y_2 - 0.254y_3 + 0.3405y_4 + 0.3405y_5 + 0.3405y_6 > -0.008855, \text{ if } y_1, y_2, y_3 \leq 2.13,$
- 8'. $-\sigma - 0.167y_1 - 0.167y_2 - 0.167y_3 - 0.0781y_4 - 0.0781y_5 - 0.0781y_6 > -1.51017,$
if $y_1, y_2, y_3 \leq 2.13.$

A.7. Branch and Bound methods.

For each case that failed the tests of A.5, we use a branch-and-bound method as follows. We pick 10 quasi-regular tetrahedra in the configuration. We divide the domain into 2^{10} cases by imposing the constraint $y_4 + y_5 + y_6 \leq 6.25$ or $y_4 + y_5 + y_6 \geq 6.25$ at each quasi-regular tetrahedron. Depending on which constraint is picked, we add (to the inequalities already present) the first group 1–7 or the second group 1'–4' of inequalities. Whenever we write of the branch-and-bound inequalities associated

with various faces, we mean these two groups of inequalities. When r faces are used, there are 2^r linear programs. Before running these we determine the maximum dihedral angles and edge lengths by separate linear programs. If the conditions of A.4.2, A.4.3 are met, we add these equations. Most of the 2^{10} linear programs give bounds under 8 pt . The only planar maps that still give bounds over 8 pt are PM(4, 126) and PM(4, 178).

A.8. Final cases.

The case PM(4, 178) is not difficult. The maximum height of a vertex is less than 2.13, by linear programming bounds. Add the inequalities from A.3 and A.6 that assume this condition. With these additional inequalities, the linear programming bound is less than 8 pt .

In the case PM(4, 126), again we find that the vertices have heights less than 2.13, and we add the relevant inequalities. The score is less than 8 pt unless the quad clusters fall into the pure Voronoi case or mixed cases. (That is, there are no flat quarters and no octahedra.) In these remaining cases the diagonals of the quad clusters are at least $2\sqrt{2}$.

Fix a vertex of type (4, 1) in the planar map. There are two such vertices to choose from, but there is an isomorphism carrying one to the other. Let v_1, v_2, v_3, v_4 be the corners of one of the quad clusters, with v_1 the chosen vertex of type (4, 1). The linear programming upper bound on the dihedral angle of the quad cluster along $(0, v_1)$ is less than 1.694. The linear programming upper bound on $|v_2| + |v_1 - v_2| + |v_1 - v_4| + |v_4|$ is less than 8.709. The following inequality, established by interval computations, implies that $|v_2 - v_4| \in [2\sqrt{2}, 2.93]$.

1. $\text{dih} > 1.694$, if $y_1, y_2, y_3 \leq 2.13$, $y_2 + y_3 + y_5 + y_6 \leq 8.709$, and $y_4 \geq 2.93$.

This allows us to add the following two interval computations to the set of linear programming inequalities. Both hold for simplices satisfying $y_1, y_2, y_3 \leq 2.13$, $y_4 \in [2\sqrt{2}, 2.93]$, $y_5, y_6 \in [2, 2.51]$. The quad cluster is broken in two simplices, with these inequalities holding on each simplex.

2. $\text{dih}_2 + 0.59y_1 + 0.1y_2 + 0.1y_3 + 0.55y_4 - 0.6y_5 - 0.12y_6 > 2.6506$.
3. $\text{dih}_2 + 0.35y_1 - 0.24y_2 + 0.05y_3 + 0.35y_4 - 0.72y_5 - 0.18y_6 < 0.47$.

With these additional inequalities, the linear programming bound drops below 8 pt . We conclude that all 18 planar maps that have scores below 8 pt . This concludes the proof of the main theorem of the paper and the third step in the proof of the Kepler conjecture.

APPENDIX 2. INTERVAL VERIFICATIONS

We make a few remarks in this appendix on the verification of the inequalities of Proposition 4.1 and 4.2. The basic method in proving an inequality $f(x) < 0$ for $x \in C$, is to use computer-based interval arithmetic to obtain rigorous upper bounds on the second derivatives: $|f_{ij}(x)| \leq a_{ij}$, for $x \in C$. These bounds lead immediately to upper bounds on $f(x)$ through a Taylor approximation with explicit bounds on the error. We divide the domain C as necessary until the Taylor approximation on each piece is less than the desired bound.

Some of the inequalities involve as many as 12 variables, such as the octahedral cases of Proposition 4.2. These are not directly accessible by computer. We describe some reductions we have used, based on linear programming. We start by applying the dimension reduction techniques described in I.8.7. We have used these whenever possible.

We will describe Proposition 4.2 because in various respects these inequalities have been the most difficult to prove, although the verifications of Propositions 4.1 and 4.3 are quite similar. If there is a diagonal of length $\leq 2\sqrt{2}$, we have two flat quarters S_1 and S_2 . The score breaks up into $\sigma = \sigma(S_1) + \sigma(S_2)$. The simplices S_1 and S_2 share a three-dimensional face. The inequality we wish to prove has the form

$$\sigma \leq a(\text{dih}(S_1) + \text{dih}_2(S_1) + \text{dih}_2(S_2)) + b.$$

We break the shared face into smaller domains on which we have

$$\begin{aligned} \sigma(S_1) &\leq a(\text{dih}(S_1) + \text{dih}_2(S_1)) + b_1, \\ \sigma(S_2) &\leq a \text{dih}_2(S_1) + b_2, \end{aligned}$$

for some b_1, b_2 satisfying $b_1 + b_2 \leq b$. These inequalities are six-dimensional verifications.

If the quad cluster is an octahedron with upright diagonal, there are four upright quarters S_1, \dots, S_4 . We consider inequalities of the form

$$(X_i) \quad \sigma(S_i) \leq \sum_{j \neq 4} a_j^i y_j(S_i) + a_7(\text{dih}_1(S_i) - \pi/2) + \sum_{j=2}^3 a \epsilon_j^i \text{dih}_j(S_i) + b^i.$$

If $\sum_{i=1}^4 a_j^i \leq 0$, $j \neq 4$, and $\sum_i b^i \leq b$, then for appropriate $\epsilon_j^i \in \{0, 1\}$, these inequalities imply the full inequality for octahedral quad clusters.

By linear programming techniques, we were able to divide the domain of all octahedra into about 1200 pieces and find inequalities of this form on each piece, giving an explicit list of inequalities that imply Proposition 4.2. The inequalities involve six variables and were verified by interval arithmetic.

To find the optimal coefficients a_j^i by linear programming we pose the linear problem

$$\begin{aligned} & \max t \\ & \text{such that} \\ & X_i, \quad i = 1, 2, 3, 4, \{S_1, S_2, S_3, S_4\} \in C \\ & \sum_i a_j^i \leq 0, \\ & \sum_i b^i \leq b, \end{aligned}$$

where $\{S_1, S_2, S_3, S_4\}$ runs over all octahedra in a given domain C . The nonlinear inequalities X_i are to be regarded as linear conditions on the coefficients a_j^i , b^i , etc. The nonlinear functions $\sigma(S_i)$, $\text{dih}(S_i)$, $y_j(S_i)$ are to be regarded as the coefficients of the variables a_j^i, \dots in a system of linear inequalities. There are infinitely many constraints, because the set C of octahedra is infinite. In practice we approximate C by a large finite set. If the maximum of t is positive, then we have a collection of inequalities in small dimensions that imply the inequality for octahedral quad clusters. Otherwise, we subdivide C into smaller domains and try again. Eventually, we succeed in partitioning the problem into six-dimensional pieces, which were verified by interval methods.

If the quad cluster is a mixed case, then [F] gives

$$\sigma \leq \text{vor}_0, -1.04 \, pt,$$

so also

$$\sigma \leq \frac{3}{4} \text{vor}_0 + \frac{1}{4}(-1.04 \, pt).$$

In the pure Voronoi case with no quarters and no enclosed vertices, we have the approximation

$$\sigma \leq \text{vor}(\cdot, \sqrt{2}) \leq \text{vor}_0.$$

If we prove $\text{vor}_0 \leq a(\text{dih}_1 + \text{dih}_2) + b$, the mixed case is established. This is how Inequality 4.2.1 was established. Dimension reduction reduces this to a seven-dimensional verification. We draw the shorter of the two diagonals between corners of the quad cluster. As we begin to subdivide this seven-dimensional domain, we are able to separate the quad cluster into two simplices along the diagonal, each scored by vor_0 . This reduces the dimension further, to make it accessible. The two cases, 4.2.2 and 4.2.3, are similar, but we establish the inequalities

$$\begin{aligned} \frac{3}{4} \text{vor}_0 + \frac{1}{4}(-1.04 \, pt) &\leq a(\text{dih}_1 + \text{dih}_2) + b, \\ \text{vor}(\cdot, \sqrt{2}) &\leq a(\text{dih}_1 + \text{dih}_2) + b. \end{aligned}$$

This completes our sketch of how the verifications were made.